HDF5: Managing Large Data Without Losing Your Mind Using the HDF5 File Format with R and Python

Jin Hyun Ju

Weill Cornell Graduate School of Medical Sciences

May 5, 2016

Caution: This talk may or may not be useful.

What I do

Expression Quantitative Trait Loci (eQTL) Analysis

- ▶ Genotype Data = $N \times 800,000$
- ▶ Phenotype Data = $N \times 20,000$
- ▶ SNP information = Chromosome, Position, ids
- Gene information = Chromosome, Start, End, id
- Covariates

Workflow

- 1. Phenotype vs Genotype association testing
- 2. Saving outcomes as a p-value matrix (around 200GB)
- Calculating False Discovery Rate etc... (needs access to the whole p-value matrix)
- 4. Identify significant associations
- Investigate significant associations using SNP and Gene information

Challenges

How can I keep information for a specific dataset in one place? (and minimize the chance of mixing up datasets...)

▶ Dealing with result files that are too big to load into memory at once

Pass data between R and Python

Primary Solution

- How can I keep information for a specific dataset in one place? Saved all the necessary objects in .RData files Can't inspect elements without loading them all into memory Only works with R
- Dealing with result files that are too big to load into memory at once
 bigmemory package: File backed matrices
 Only works with R
- Pass data between R and Python Temporary text files
 Unnecessary data duplication
 Uneasy feeling of creating waste

Solution

Hierarchical Data Format 5 (HDF5)

- Folder like structures inside a single file Can hold various kinds of data
- Can get an overview of the contents
 Inspect elements without loading everything into memory
- Customizable structure
 Can create a structure that is convenient for the user
- Compression and chunking features available
 Fine tune I/O and storage space
- ► Fully compatible with R and Python Environment friendly